

=> file hcaplus  
FILE 'HCAPLUS' ENTERED AT 15:23:11 ON 17 JUL 2007  
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FILE COVERS 1907 - 17 Jul 2007 VOL 147 ISS 4  
FILE LAST UPDATED: 16 Jul 2007 (20070716/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos 144

L40	439	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	SAVAGE P?/AU
L41	85	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	BENDELAC A?/AU
L42	103	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	TEYTON L?/AU
L43	20	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L40 AND L41 AND L42
L44	5	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L43 AND (1840-2003)/PRY, PY,AY

=> d ibib ed abs 144 1-5

L44 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:927222 HCAPLUS

DOCUMENT NUMBER: 141:350362

TITLE: Synthesis and NKT Cell Stimulating Properties of Fluorophore- and Biotin-Appended 6''-Amino-6''-deoxy-galactosylceramides.

INVENTOR(S): Savage, Paul B.; Bendelac, Albert; Teyton, Luc

PATENT ASSIGNEE(S): Brigham Young University, USA

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004094444	A1	20041104	WO 2003-US8530	

200303  
20

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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2519568 A1 20041104 CA 2003-2519568

200303  
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AU 2003225891 A1 20041119 AU 2003-225891

200303  
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EP 1611147 A1 20060104 EP 2003-816701

200303  
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

US 2006264382 A1 20061123 US 2005-550165

200509  
20

PRIORITY APPLN. INFO.:

WO 2003-US8530

W

200303  
20

OTHER SOURCE(S): MARPAT 141:350362

ED Entered STN: 04 Nov 2004

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB  $\alpha$ -Galactosylceramides I, wherein R1 is H, substituted sulfonyl; R1R2 together form heterocycle; R2 is H; R3-R7 are independently H, alkyl, aralkyl, acyl; R8 is (CH<sub>2</sub>)<sub>x</sub>Me; x is 1-100; R9 is alkyl; are potent stimulators of human T cells. Stimulation occurs through binding of the glycolipids by CD1d, presentation to T cells, and formation of a CD1D-glycolipid-T cell receptor complex. To facilitate the elucidation of the structural features of glycolipids necessary for T cell stimulation,  $\alpha$ -galactosylceramides have been prepared with small mols. appended at the C6 position of the sugar. The appended mols. do not significantly influence the abilities of the glycolipids to stimulate T cells. Thus, galactosylceramide II was prepared and tested in mice in stimulating NKT cells.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:306445 HCAPLUS

DOCUMENT NUMBER: 138:400350

TITLE: The Paradox of Immune Molecular Recognition of  $\alpha$ -Galactosylceramide: Low Affinity, Low Specificity for CD1d, High Affinity for  $\alpha\beta$  TCRs

AUTHOR(S): Cantu, Carlos, III; Benlagha, Kamel; Savage, Paul B.; Bendelac, Albert; Teyton, Luc

CORPORATE SOURCE: Department of Immunology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Journal of Immunology (2003), 170(9), 4673-4682

CODEN: JOIMA3; ISSN: 0022-1767

PUBLISHER: American Association of Immunologists

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 22 Apr 2003

AB CD1 resembles both class I and class II MHC but differs by the important aspect of presenting lipid/glycolipids, instead of peptides, to T cells. Biophys. studies of lipid/CD1 interactions have been limited, and kinetics of binding are in contradiction with functional studies. We have revisited this issue by designing new assays to examine the loading of CD1 with lipids. As expected for hydrophobic interactions, binding affinity was not high and had limited specificity. Lipid critical micelle concentration set the limitation to these studies. Once loaded onto CD1d, the recognition of glycolipids by  $\alpha\beta$  T cell receptor was studied by surface plasmon resonance using soluble V $\alpha$ 14-V $\beta$ 8.2 T cell receptors. The V $\alpha$ 14 J $\alpha$ 18 chain could be paired with NK1.1 cell-derived V $\beta$  chain, or any V $\beta$ 8 chain, to achieve high affinity recognition of  $\alpha$ -galactosylceramide. Biophys. anal. indicated little effect of temperature or ionic strength on the binding interaction, in contrast to what has been seen in peptide/MHC-TCR studies. This suggests that there is less accommodation made by this TCR in recognizing  $\alpha$ -galactosylceramide, and it can be assumed that the most rigid part of the Ag, the sugar moiety, is critical in the interaction.

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:318756 HCAPLUS

TITLE: Lipid presentation by CD1: the short and the long lipid story

AUTHOR(S): Bendelac, A.; Teyton, L.; Savage, P. B.

CORPORATE SOURCE: Department of Molecular Biology, Princeton University, Princeton, NJ, 08544, USA

SOURCE: Nature Immunology (2002), 3(5), 421-422

CODEN: NIAMCZ; ISSN: 1529-2908

PUBLISHER: Nature America Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 29 Apr 2002

AB Unavailable

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN  
THE RE FORMAT

L44 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2002:207112 HCAPLUS  
DOCUMENT NUMBER: 136:369933  
TITLE: Synthesis and NKT Cell Stimulating Properties of  
Fluorophore- and Biotin-Appended  
6''-Amino-6''-deoxy-galactosylceramides  
AUTHOR(S): Zhou, Xiao-Ti; Forestier, Claire; Goff, Randal  
D.; Li, Chunhong; Teyton, Luc;  
Bendelac, Albert; Savage, Paul  
B.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry,  
Brigham Young University, Provo, UT, 84602, USA  
SOURCE: Organic Letters (2002), 4(8),  
1267-1270  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 136:369933

ED Entered STN: 20 Mar 2002

AB  $\alpha$ -Galactosylceramides are potent stimulators of human T cells.  
Stimulation occurs through binding of the glycolipids by CD1d,  
presentation to T cells, and formation of a CD1d-glycolipid-T cell  
receptor complex. To facilitate the elucidation of the structural  
features of glycolipids necessary for T cell stimulation,  
 $\alpha$ -galactosylceramides have been prepared with small mols.  
appended at the C6 position of the sugar. The appended mols. do not  
significantly influence the abilities of the glycolipids to  
stimulate T cells.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L44 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2002:43462 HCAPLUS  
DOCUMENT NUMBER: 136:230865  
TITLE: Multiple defects in antigen presentation and T  
cell development by mice expressing cytoplasmic  
tail-truncated CD1d  
AUTHOR(S): Chiu, Ya-Hui; Park, Se-Ho; Benlagha, Kamel;  
Forestier, Claire; Jayawardena-Wolf, Jayanthi;  
Savage, Paul B.; Teyton, Luc;  
Bendelac, Albert  
CORPORATE SOURCE: Department of Molecular Biology, Princeton  
University, Princeton, NJ, 08544, USA  
SOURCE: Nature Immunology (2002), 3(1), 55-60  
CODEN: NIAMCZ; ISSN: 1529-2908  
PUBLISHER: Nature America Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

ED Entered STN: 17 Jan 2002

AB For members of the CD1 family of  $\beta$ 2-microglobulin-associated  
lipid-presenting mols., tyrosine-based motifs in the cytoplasmic  
tail and invariant chain (Ii) govern glycoprotein trafficking  
through endosomal compartments. Little is known about the  
intracellular pathways of CD1 trafficking and antigen presentation.

However, in vitro studies with cells transfected with mutant CD1 that had a truncated cytoplasmic tail have suggested a role for these tyrosine motifs in some, but not all, antigenic systems. By introducing a deletion of the tyrosine motif into the germ line, and through homologous recombination in embryonic stem cells, we now describe knock-in mice with the CD1d cytoplasmic tail deleted. Despite adequate surface CD1d expression and the presence of Ii, these mutant mice showed multiple and selective abnormalities in intracellular trafficking, antigen presentation and T cell development, demonstrating the critical functions of the CD1d cytoplasmic tail motif in vivo.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

=> d his nofile

(FILE 'HOME' ENTERED AT 12:09:06 ON 17 JUL 2007)

FILE 'HCAPLUS' ENTERED AT 12:09:20 ON 17 JUL 2007

E US20060264382/PN

L1 1 SEA ABB=ON PLU=ON US2006264382/PN  
SEL RN

FILE 'REGISTRY' ENTERED AT 12:09:41 ON 17 JUL 2007

L2 19 SEA ABB=ON PLU=ON (158021-47-7/BI OR 205371-68-2/BI OR  
217176-82-4/BI OR 35013-72-0/BI OR 424823-18-7/BI OR  
424823-19-8/BI OR 424823-20-1/BI OR 424823-22-3/BI OR  
424823-23-4/BI OR 424823-24-5/BI OR 424823-25-6/BI OR  
424823-26-7/BI OR 424823-27-8/BI OR 424823-28-9/BI OR  
424823-29-0/BI OR 424823-30-3/BI OR 4711-00-6/BI OR  
605-65-2/BI OR 88714-17-4/BI)

FILE 'HCAPLUS' ENTERED AT 12:09:50 ON 17 JUL 2007

L3 1 SEA ABB=ON PLU=ON L1 AND L2

FILE 'REGISTRY' ENTERED AT 12:23:36 ON 17 JUL 2007

L36 STRUCTURE  
L37 0 SEA SSS SAM L36  
L38 17 SEA SSS FUL L36  
SAV L38 KRI165/A

FILE 'HCAPLUS' ENTERED AT 15:11:35 ON 17 JUL 2007

L39 8 SEA ABB=ON PLU=ON L38  
L40 439 SEA ABB=ON PLU=ON SAVAGE P?/AU  
L41 85 SEA ABB=ON PLU=ON BENDELAC A?/AU  
L42 103 SEA ABB=ON PLU=ON TEYTON L?/AU  
L43 20 SEA ABB=ON PLU=ON L40 AND L41 AND L42  
L44 5 SEA ABB=ON PLU=ON L43 AND (1840-2003)/PRY,PY,AY  
L45 6 SEA ABB=ON PLU=ON L39 NOT L44

FILE 'HCAPLUS' ENTERED AT 15:23:11 ON 17 JUL 2007

D QUE NOS L44  
D IBIB ED ABS L44 1-5

=> file reg

FILE 'REGISTRY' ENTERED AT 15:23:37 ON 17 JUL 2007

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 JUL 2007 HIGHEST RN 942468-13-5

DICTIONARY FILE UPDATES: 16 JUL 2007 HIGHEST RN 942468-13-5

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

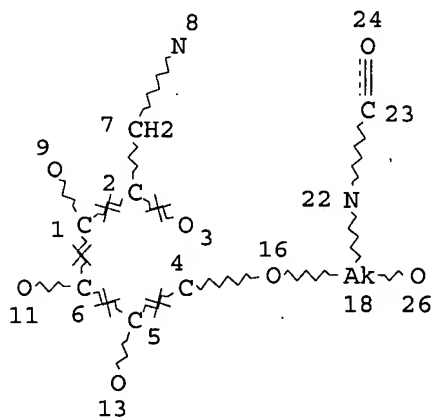
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> d stat que l38

L36 STR



NODE ATTRIBUTES:

NSPEC IS RC AT 3

NSPEC IS RC AT 4

NSPEC IS RC AT 8

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 18

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L38 17 SEA FILE=REGISTRY SSS FUL L36

100.0% PROCESSED 332123 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.08

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FILE 'HCAPLUS' ENTERED AT 15:23:48 ON 17 JUL 2007  
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FILE COVERS 1907 - 17 Jul 2007 VOL 147 ISS 4  
FILE LAST UPDATED: 16 Jul 2007 (20070716/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos 145

L36	STR
L38	17 SEA FILE=REGISTRY SSS FUL L36
L39	8 SEA FILE=HCAPLUS ABB=ON PLU=ON L38
L40	439 SEA FILE=HCAPLUS ABB=ON PLU=ON SAVAGE P?/AU
L41	85 SEA FILE=HCAPLUS ABB=ON PLU=ON BENDELAC A?/AU
L42	103 SEA FILE=HCAPLUS ABB=ON PLU=ON TEYTON L?/AU
L43	20 SEA FILE=HCAPLUS ABB=ON PLU=ON L40 AND L41 AND L42
L44	5 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 AND (1840-2003)/PRY, PY,AY
L45	6 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 NOT L44

=> d ibib ed abs hitstr 145 1-6

L45 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2007:463101 HCAPLUS  
DOCUMENT NUMBER: 146:440188  
TITLE: Hexosylceramides as adjuvants and their uses in  
pharmaceutical compositions  
INVENTOR(S): Ebensen, Thomas; Morr, Michael; Guzman, Carlos  
A.  
PATENT ASSIGNEE(S): GBF Gesellschaft fuer Biotechnologische  
Forschung MbH, Germany  
SOURCE: PCT Int. Appl., 61pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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Ross Shipe EIC 1600 Remsen 4B71 571-272-6018

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WO 2007045469

A1

20070426

WO 2006-EP10086

200610  
19

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

EP 1776963

A1

20070425

EP 2005-22771

200510  
19

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU

PRIORITY APPLN. INFO.:

EP 2005-22771

A

200510  
19

OTHER SOURCE(S): MARPAT 146:440188

ED Entered STN: 27 Apr 2007

AB The present invention relates to new adjuvants and the uses in pharmaceutical compns., like in vaccines. In particular, the present invention provides new compds. useful as adjuvants for prophylactic and/or therapeutic vaccination in the treatment of infectious diseases, inflammatory diseases, autoimmune diseases, tumors, allergies as well as for the control of fertility in human or animal populations. The compds. are particularly useful not only as systemic, but preferably as mucosal adjuvants. In addition, the invention relates to its uses as active ingredients in pharmaceutical compns.

IT 934480-71-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

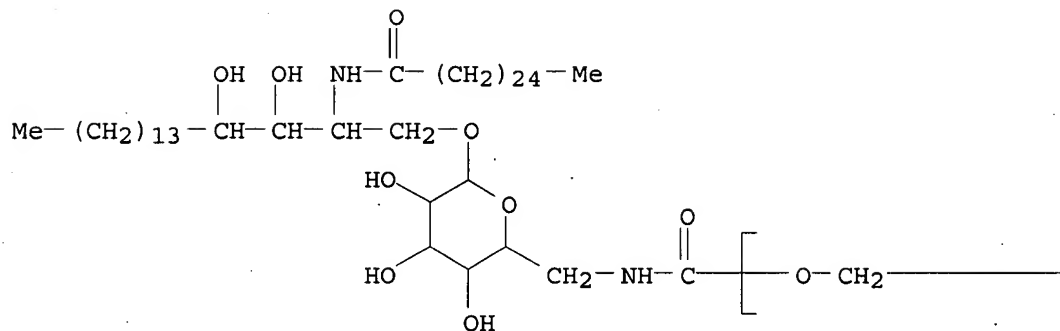
(hexosylceramides as adjuvants and their use in vaccines)

RN 934480-71-4 HCAPLUS

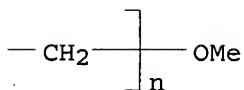
CN Poly(oxy-1,2-ethanediyl),  $\alpha$ -hydro- $\omega$ -methoxy-, ester with N-[(1S,2S,3R)-1-[[[6-(carboxyamino)-6-deoxy- $\alpha$ -D-galactopyranosyl]oxy)methyl]-2,3-dihydroxyheptadecyl]hexacosanamide (CA INDEX NAME)



PAGE 1-A



PAGE 1-B



IT. 424823-29-0

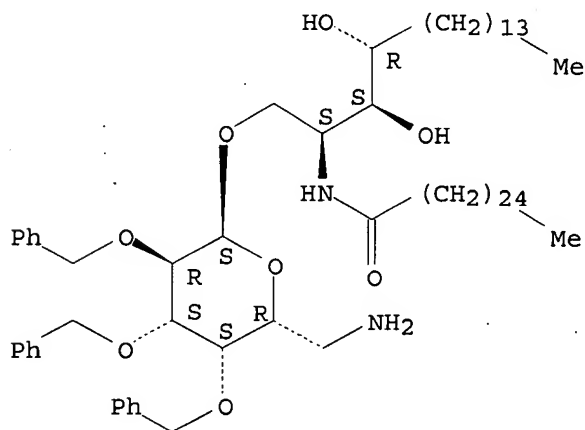
RL: RCT (Reactant); RACT (Reactant or reagent)

(hexosylceramides as adjuvants and their use in vaccines)

RN 424823-29-0 HCAPLUS

CN Hexacosanamide, N-[(1S,2S,3R)-1-[[[6-amino-6-deoxy-2,3,4-tris-O-(phenylmethyl)-α-D-galactopyranosyl]oxy]methyl]-2,3-dihydroxyheptadecyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 934480-72-5P

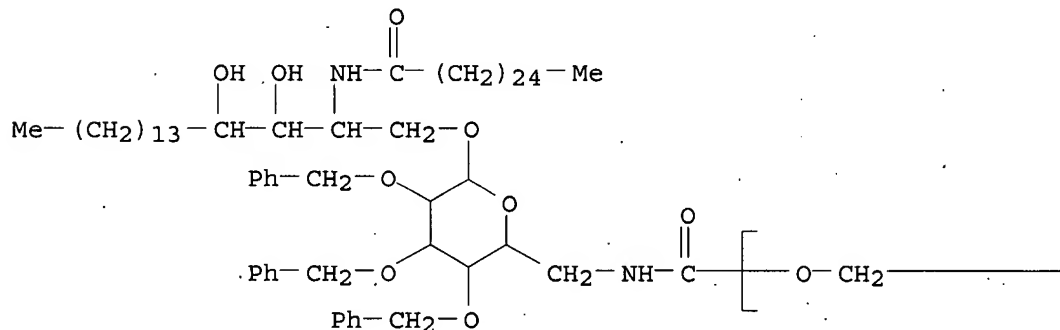
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)

(hexosylceramides as adjuvants and their use in vaccines)

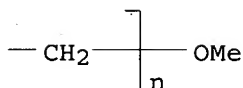
RN 934480-72-5 HCAPLUS

CN Poly(oxy-1,2-ethanediyl),  $\alpha$ -hydro- $\omega$ -methoxy-, ester with  
 N-[(1S,2S,3R)-1-[[[6-(carboxyamino)-6-deoxy-2,3,4-tris-O-  
 (phenylmethyl)- $\alpha$ -D-galactopyranosyl]oxy)methyl]-2,3-  
 dihydroxyheptadecyl]hexacosanamide (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN  
 THE RE FORMAT

L45 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:533879 HCAPLUS

DOCUMENT NUMBER: 145:143203

TITLE: A modified  $\alpha$ -galactosyl ceramide for  
 staining and stimulating natural killer T cells

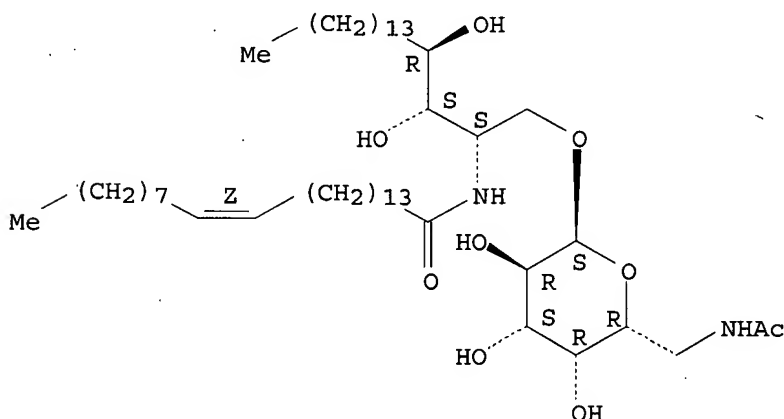
AUTHOR(S): Liu, Yang; Goff, Randal D.; Zhou, Dapeng;  
 Mattner, Jochen; Sullivan, Barbara A.; Khurana,  
 Archana; Cantu, Carlos; Ravkov, Eugene V.;  
 Ibegbu, Chris C.; Altman, John D.; Teyton, Luc;  
 Bendelac, Albert; Savage, Paul B.

CORPORATE SOURCE: Brigham Young University, Provo, UT, 84602, USA  
 SOURCE: Journal of Immunological Methods (2006),  
 312(1-2), 34-39

PUBLISHER: CODEN: JIMMBG; ISSN: 0022-1759  
 Elsevier B.V.

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 07 Jun 2006  
 AB CD1d presentation of  $\alpha$ -galactosyl ceramides to natural killer T cells has been a focal point of the study of regulatory T cells. KRN7000, an  $\alpha$ -galactosyl ceramide originally generated from structure activity studies of antitumor properties of marine sponge glycolipids, is currently the most commonly used agonist ligand and is used to stain NKT cells. However, this glycolipid suffers from poor solubility and availability. The authors have developed an  $\alpha$ -galactosyl ceramide with improved solubility over KRN7000 that effectively stains NKT cells, both mouse and human, and stimulates cytokine release at low concns.  
 IT 898531-99-2, PBS 57  
 RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)  
 (α-galactosyl ceramide ligand for staining and stimulation of NK T-cells)  
 RN 898531-99-2 HCAPLUS  
 CN 15-Tetracosenamide, N-[(1S,2S,3R)-1-[[[6-(acetylamino)-6-deoxy-α-D-galactopyranosyl]oxy]methyl]-2,3-dihydroxyheptadecyl]-, (15Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:523485 HCAPLUS

DOCUMENT NUMBER: 141:257202

TITLE: Phylogeny of the ring-forming bacterium *Arcicella aquatica* gen. nov., sp. nov. (ex Nikitin et al. 1994), from a freshwater neuston biofilm

AUTHOR(S): Nikitin, Denis I.; Stroempl, Carsten; Oranskaya, M. S.; Abraham, Wolf-Rainer

CORPORATE SOURCE: Institute of Microbiology, Russian Academy of Sciences, Moscow, 117811, Russia

SOURCE: International Journal of Systematic and Evolutionary Microbiology (2004), 54(3), 681-684

CODEN: ISEMF5; ISSN: 1466-5026  
 PUBLISHER: Society for General Microbiology  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

ED Entered STN: 30 Jun 2004

AB *Arcicella aquatica* NO-502T, obtained from a neuston film on a freshwater lake and belonging to the phylum Bacteroidetes, is characterized by ring-forming cells. The bacterium is a strict aerobe, with optimal growth between 28 and 30°. Carbohydrates, but no organic acids or amino acids, are used as substrates. The G+C content of strain NO-502T is 34.5 mol%; its genome size is 2.9+109 Da. The genus *Arcicella* and its type species *Arcicella aquatica* (type strain NO-502T=LMG 21963T=CIP 107990T) are proposed, and descriptions of this genus and species are given.

IT 251095-67-7

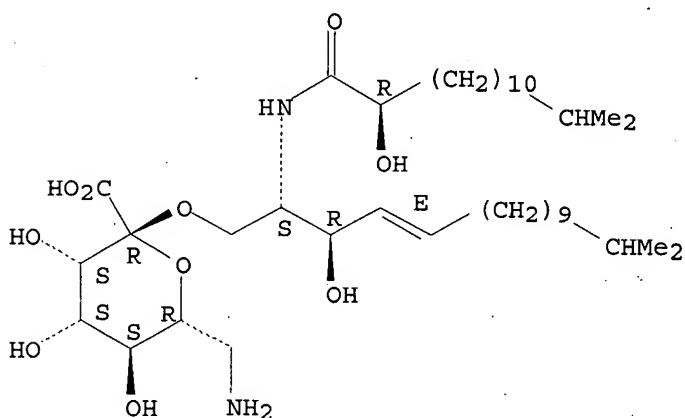
RL: BSU (Biological study, unclassified); BIOL (Biological study) (phylogeny and biochem. characterization of ring-forming bacterium *Arcicella aquatica* from a freshwater neuston biofilm based on rDNA sequences and polar lipids)

RN 251095-67-7 HCAPLUS

CN  $\alpha$ -D-manno-2-Heptulopyranosidonic acid, (2S,3R,4E)-3-hydroxy-2-[[[(2R)-2-hydroxy-13-methyl-1-oxotetradecyl]amino]-15-methyl-4-hexadecenyl 7-amino-7-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:132275 HCAPLUS

DOCUMENT NUMBER: 136:356788

TITLE: Regioselective reaction of unprotected sugars with urethane N-carboxyanhydrides for the synthesis of new surfactants

AUTHOR(S): Bellhaouel, Salima; Roumestant, Marie-Louise; Viallefont, Philippe; Martinez, Jean

CORPORATE SOURCE: UMR 5810-CNRS Laboratoire des Amino Acides, Peptides et Proteines, Montpellier, 34095, Fr..

SOURCE: Synthetic Communications (2002), 32(2), 181-187

CODEN: SYNCAV; ISSN: 0039-7911

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 20 Feb 2002

AB Reaction of urethane N-carboxyanhydrides with unprotected amino sugars was the key step in the synthesis of new trimodular surfactants. Reaction of a 2:1 mixture of N-methylglucamine with the N-BOC derivative of 4-methyl-1,3-oxazoline-2,5-dione in DMF at room temperature gave a 36% yield of N-[(2-BOC-amino)propionyl]-N-methylglucamine.

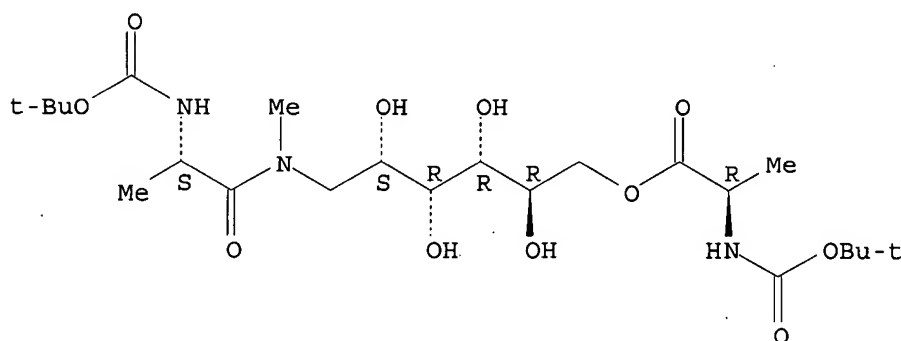
IT 420132-49-6P 420132-50-9P 420132-51-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(regioselective reaction of unprotected sugars with urethane N-carboxyanhydrides for synthesis of new surfactants)

RN 420132-49-6 HCAPLUS

CN L-Alanine, N-[(1,1-dimethylethoxy)carbonyl]-, 6-ester with  
1-deoxy-1-[[[(2S)-2-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxopropyl]methylamino]-D-glucitol (9CI) (CA INDEX NAME)

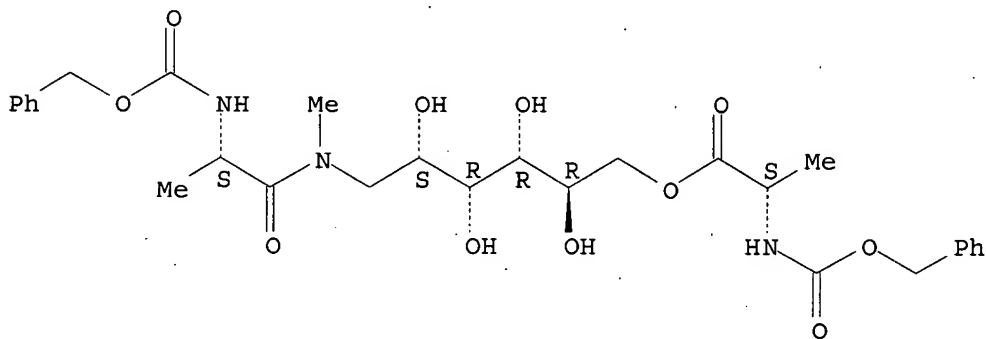
Absolute stereochemistry.



RN 420132-50-9 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-, 6-ester with  
1-deoxy-1-[methyl[(2S)-1-oxo-2-[[[(phenylmethoxy)carbonyl]amino]propyl]amino]-D-glucitol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



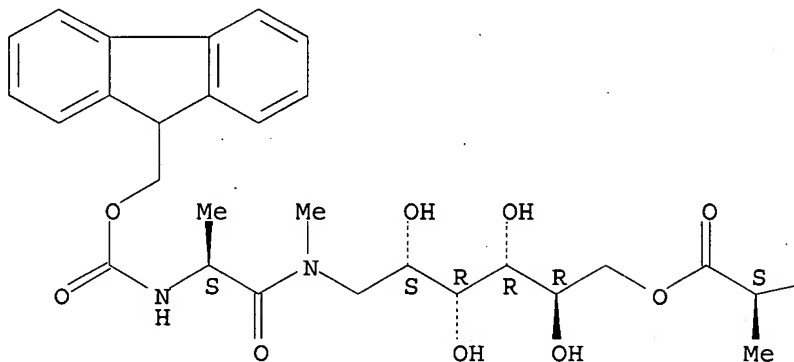
RN 420132-51-0 HCAPLUS

CN L-Alanine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-, 6-ester with  
1-deoxy-1-[[[(2S)-2-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-oxopropyl]methylamino]-D-glucitol (9CI) (CA INDEX NAME)

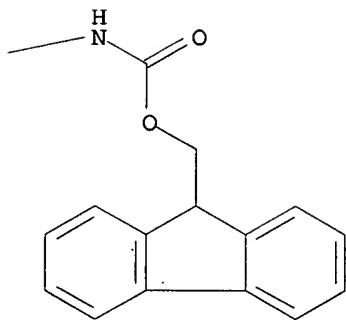
oxopropyl]methylamino]-D-glucitol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

11

THERE ARE 11 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L45 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:584460 HCAPLUS

DOCUMENT NUMBER: 132:1853

TITLE: A novel glycosphingolipid from Gram-negative aquatic bacteria

AUTHOR(S): Batrakov, S. G.; Sheichenko, V. I.; Nikitin, D. I.

CORPORATE SOURCE: Research Centre 'Hydrobios' of Ministry of Health, Moscow, Russia

SOURCE: Biochimica et Biophysica Acta, Molecular and

Cell Biology of Lipids (1999), 1440(2-3),  
163-175

CODEN: BBMLFG; ISSN: 1388-1981

PUBLISHER:

Elsevier B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

ED Entered STN: 17 Sep 1999

AB The chloroform-methanol extractable lipids of the Gram-neg. fresh-water bacteria *Arcocella aquatica* NO-502 and *Flectobacillus* major FM were found to contain an unusual ninhydrin-pos. glycolipid. It was purified by two-stage silica gel-column chromatog. By the use of IR and <sup>1</sup>H-NMR spectroscopy, mass spectrometry and chemical-degradation experiment, the lipid was established to be 1-O-monoglycosyl ceramide, the carbohydrate moiety of which was the α-pyranose-ring form of 7-desoxy-7-amino-D-manno-heptulosonic acid, or 1-hydroxycarbonyl-6-deoxy-6-amino-α-D-mannopyranose. The ceramide portion consisted mainly (by 95% in the *A. aquatica* glycolipid and 80% in the *F. major* glycolipid) of 2-N-(2'-D-hydroxy-13'-methyltetradecanoyl)-15-methyl-4(E)-hexadecasphingene. The minor mol. species differed from the major one only in fatty acid structure. The glycolipid accounted for 8 and 11% of the total lipids extracted from *A. aquatica* NO-502 and *F. major* FM cells, resp.

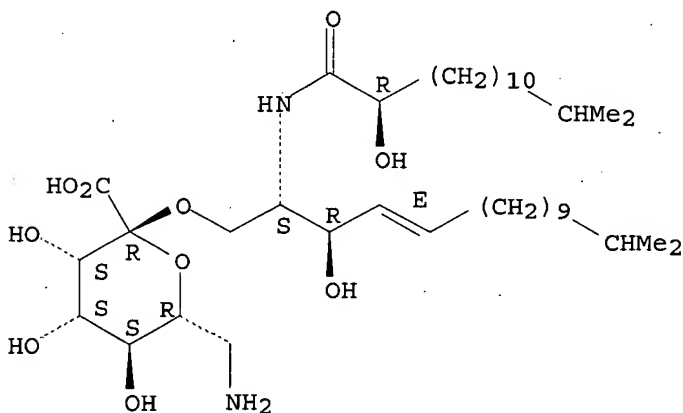
IT 251095-67-7P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (novel glycosphingolipid from Gram-neg. aquatic bacteria)

RN 251095-67-7 HCAPLUS

CN α-D-manno-2-Heptulopyranosidonic acid, (2S,3R,4E)-3-hydroxy-2-[[[(2R)-2-hydroxy-13-methyl-1-oxotetradecyl]amino]-15-methyl-4-hexadecenyl 7-amino-7-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



REFERENCE COUNT:

23 THERE ARE 23 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L45 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:359192 HCAPLUS

DOCUMENT NUMBER: 127:81767

TITLE: Internally quenched fluorogenic,  $\alpha$ -helical dimeric peptides and glycopeptides for the evaluation of the effect of glycosylation on the conformation of peptides

AUTHOR(S): Mehta, Seema; Meldal, Morten; Ferro, Vito; Duus, Jens O.; Bock, Klaus

CORPORATE SOURCE: Department of Chemistry, Carlsberg Laboratory, Copenhagen, DK-2500, Den.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (9), 1365-1374  
CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 09 Jun 1997

AB A panel of  $\alpha$ -helical, dimeric coiled-coil peptides has been designed and synthesized for the evaluation of the effect of glycosylation on the conformation of these coiled-coil peptides. Two glycosylated building blocks, N $\alpha$ -(fluoren-9-ylmethoxycarbonyl)-O-(2,3,4-tri-O-acetyl-6-azido-6-deoxy- $\beta$ -D-glucopyranosyl)-L-threonine pentafluorophenyl ester and N $\alpha$ -(fluoren-9-ylmethoxycarbonyl)-O-{2,3,4-tri-O-acetyl-6-[2'-(tert-butoxycarbonylamino)benzoylamino]-6-deoxy- $\beta$ -D-glucopyranosyl}-L-threonine pentafluorophenyl ester containing the fluorogenic 2-aminobenzamide (Abz) group, have been synthesized. These compds. have been obtained by the glycosylation of N $\alpha$ -Fmoc-Thr-OPfp with the corresponding glycosyl trichloroacetamidate donors and have been incorporated into the solid-phase synthesis of the peptides and glycopeptides. Five compds. have been synthesized as internally quenched fluorogenic compds. where the Abz group has been employed as the fluorogenic probe and 3-nitrotyrosine Tyr(NO<sub>2</sub>) as the quenching chromophore. Steady-state fluorescence studies have provided evidence to support the dimerization of the  $\alpha$ -helical peptides. Denaturation studies, by fluorescence as well as CD spectroscopy, indicate that the introduction of a carbohydrate moiety into the coiled-coil peptides has a significant destabilizing effect on the  $\alpha$ -helicity.

IT 191668-75-4P 191668-76-5P

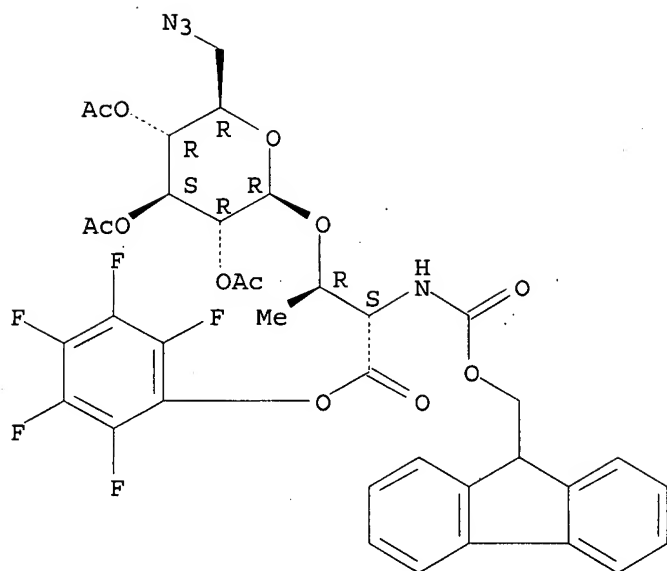
RL: SPN (Synthetic preparation); PREP (Preparation)  
(internally quenched fluorogenic, helical dimeric peptides and glycopeptides for evaluation of effect of glycosylation on conformation of peptides)

RN 191668-75-4 HCAPLUS

CN L-Threonine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-O-(2,3,4-tri-O-acetyl-6-azido-6-deoxy- $\beta$ -D-glucopyranosyl)-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



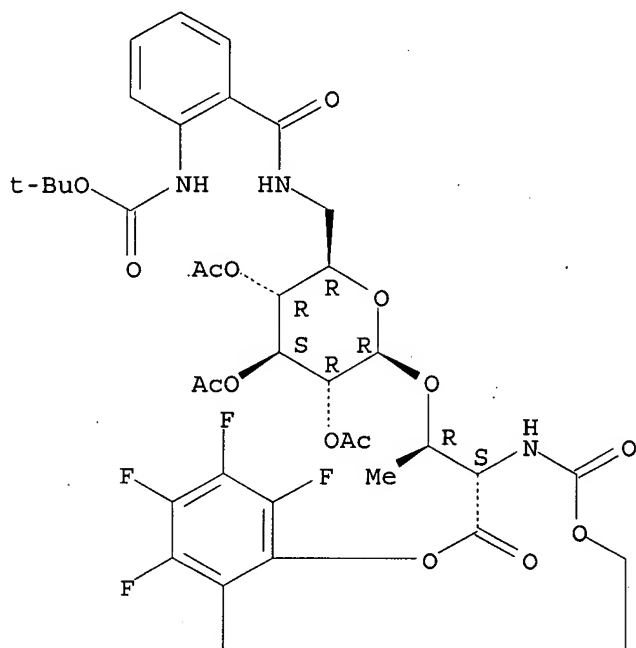


RN 191668-76-5 HCAPLUS

CN L-Threonine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-O-[2,3,4-tri-O-acetyl-6-deoxy-6-[[2-[[[(1,1-dimethylethoxy)carbonyl]amino]benzoyl]amino]-β-D-glucopyranosyl]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

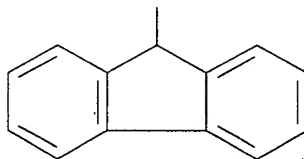
Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A

F



REFERENCE COUNT:

46

THERE ARE 46 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

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